Electronic parameters for isotope shifts of the $4s - 4p_{3/2}$ transition in Cu I

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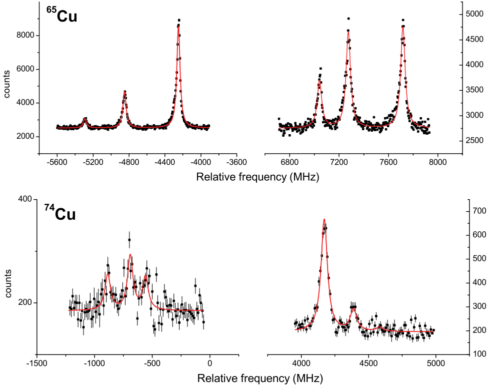
Introduction

$$IS(65, A) \equiv \nu_k^A - \nu_k^{65} = M_k \left(\frac{A - 65}{65A} \right) + F_k \, \delta \langle r^2 \rangle^{65,A}$$



Vingerhoets, PhD thesis 2011

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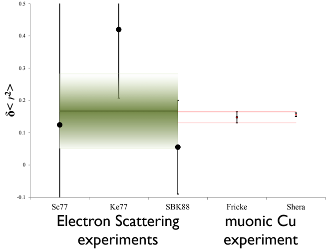
Table 6.4: Isotope shifts (IS) and differences in mean square charge radii extracted using the semi-empirical (SE) approach and ab initio calculations (AI).

Isotope	I^π	IS (MHz)	$\delta < r^2 >_{SE}$ (fm^2)	$\delta < r^2 >_{AI}$ (fm^2)
^{58}Cu	1^+	-1975(10)	-0.830(10)	0.270(15)
^{59}Cu	$3/2^-$	-1717(7)	-0.645(7)	0.306(11)
^{60}Cu	2^+	-1415(6)	-0.520(6)	0.262(9)
^{61}Cu	$3/2^-$	-1188(7)	-0.374(5)	0.257(8)
^{62}Cu	1^+	-825(4)	-0.299(4)	0.157(6)
^{63}Cu	$3/2^-$	-576.1(11)	-0.1601(12)	0.1544(17)
^{64}Cu	1^+	-249(2)	-0.114(2)	0.025(3)
^{65}Cu	$3/2^-$			
^{66}Cu	1^+	305(3)	0.046(4)	-0.118(5)
^{67}Cu	$3/2^-$	561(4)	0.131(4)	-0.174(5)
^{68}Cu	1^+	859(4)	0.163(4)	-0.300(6)
^{68}Cu	6^-	813(3)	0.212(3)	-0.231(4)
^{69}Cu	$3/2^-$	1079(2)	0.266(2)	-0.321(3)
^{70}Cu	1^+	1307(8)	0.352(9)	-0.361(13)
^{70}Cu	3^-	1335(8)	0.323(9)	-0.402(13)
^{70}Cu	6^-	1347(2)	0.310(2)	-0.420(4)
^{71}Cu	$3/2^-$	1526(9)	0.437(10)	0.-0.397(14)
^{72}Cu	2^-	1787(4)	0.471(4)	-0.503(6)
^{73}Cu	$3/2^-$	1984(12)	0.563(13)	-0.521(18)
^{74}Cu	2^-	2260(14)	0.563(15)	-0.67(2)
^{75}Cu	$5/2^-$	2484(16)	0.611(17)	-0.74(2)

Vingerhoets, PhD thesis 2011

$$\delta\langle r^2\rangle^{63,65}$$



Mark Bissel, private comm.

The MCDF method (implemented in the GRASP package)

Wave function expansion: CSF defined on optimized spinors

$$\Psi(JM_J\pi)$$

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Wave function expansion: CSF defined on optimized spinors

$$\Psi(JM_J\pi) = \sum_{i=1}^{N_c} c_i \Phi(\{\phi_{n\kappa m}\}; \gamma_i JM_J\pi)$$

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$$\phi_{n\kappa m} = \frac{1}{r} \begin{pmatrix} P_{n\kappa}(r)\,\chi_{\kappa m}(\theta,\varphi) \\ iQ_{n\kappa}(r)\,\chi_{-\kappa m}(\theta,\varphi) \end{pmatrix}$$

where κ is defined as

$$\kappa = \begin{cases} -l-1 & \text{when} \quad j = l+1/2 \\ l & \text{when} \quad j = l-1/2\,. \end{cases}$$

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Variational principle on the Dirac-Coulomb Hamiltonian

$$H_{DC} = \sum_{i}^{N} \left(c\,\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + (\beta_i - 1)c^2 + V_i^{nuc} \right) + \sum_{i>j} 1/r_{ij}$$

Systematic increase of model space

⇒ Model space in “2D”

$$\Phi_i(\gamma_i\ J\pi) \in \text{ MR-I}$$

$$\Leftrightarrow$$

$$\exists \Phi_k(\gamma_i\ J\pi) \in \text{ MR } \text{ with } \langle \gamma_i\ J\pi | H_{DC} | \gamma_k\ J\pi \rangle \neq 0 \quad \forall \{\phi_{n\kappa m}\}$$

- first-order interacting CSF defined in an *active sets* (MR-I),

  $\{\phi_{n\kappa m}\}$ chosen with $n < n_{max}$ and $l < l_{max}$

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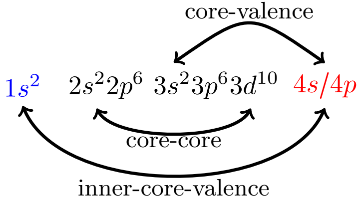
- *zero-order multi-reference*

  MR extended by including Φ_k in a specific order

Computation of F factor



model	# CSF $4s$	# CSF $4p_{3/2}$	$\tilde{\nu}$ [cm^{-1}]	F [MHz/fm^2]
DF	1	1	25 679	−597
+ C–C	1 000	1 095	25 745	−662
+ C–V	8 700	15 503	29 885	−766
+ IC–V	9 465	16 828	29 887	−775
+ high order	1 154 152	852 797	30 751	−772
Fritzsche[2]			29 244	−680(102)
Johnson *et al.* [1]			31 574	
experiment			30 784	

[1] Johnson *et al.* PRA 42 (1990) 1087

[2] unpublished

Experimental mass factors

$$\delta\nu_k^{A,A'} = M_k \left(\frac{A' - A}{AA'}\right) + F_k\, \delta\langle r^2\rangle^{A,A'}$$

With

$$\begin{aligned} \delta\nu_k^{63,65} &= 576.1 \text{ MHz} \\ F_k &= -772 \text{ Mhz/fm}^2 \\ \delta\langle r^2\rangle^{63,65} &= 0.15(2) \text{ fm}^2 \ (\mu) \\ \delta\langle r^2\rangle^{63,65} &= 0.17(12) \text{ fm}^2 \ (\text{e}^- \text{ scat.}) \end{aligned}$$

$M_k = 1417(32)$ GHz u (μ), $M_k = 1448(190)$ GHz u (ES)

Relativistic mass shifts

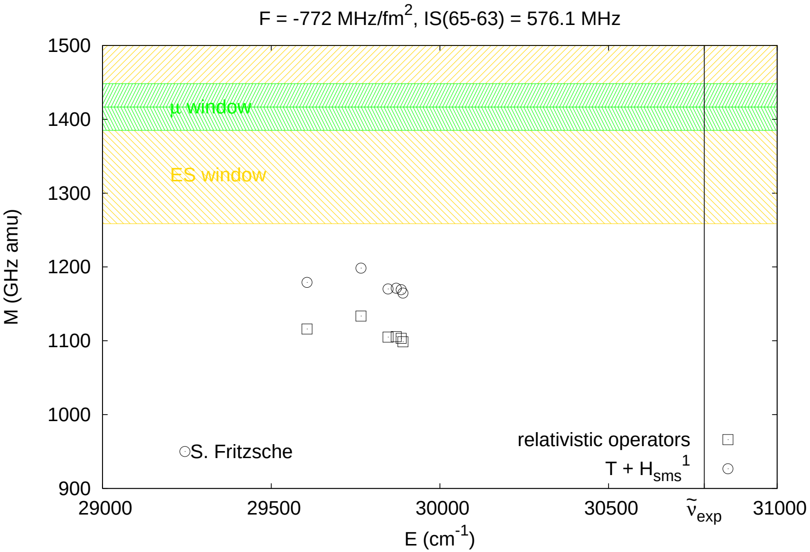
$$IS(65,A) \equiv \nu_k^A - \nu_k^{65} = M_k \left(\frac{A-65}{65A}\right) + F_k \, \delta\langle r^2\rangle^{65,A}$$

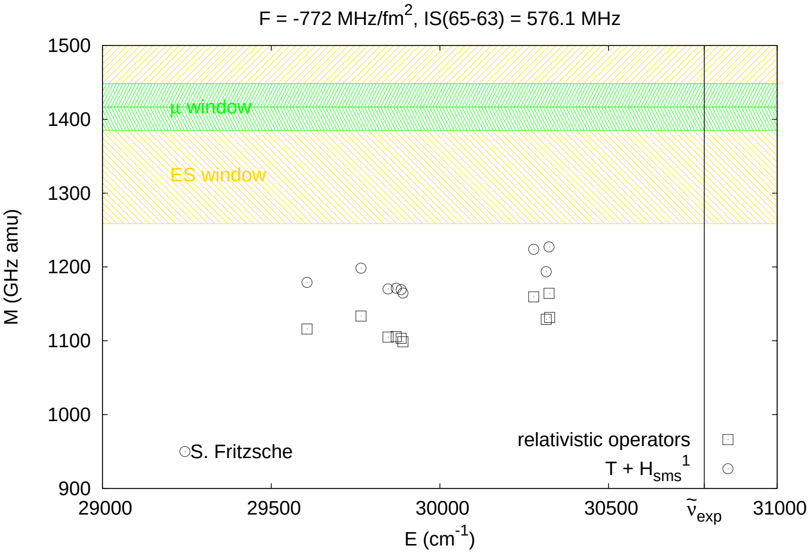
$$M_k \rightarrow H_{\mathrm{NMS}} + H_{\mathrm{SMS}}$$

Relativistic effects on the mass isotope shift

$$H_{\mathrm{NMS}} = \frac{1}{2M}\sum_{i=1}^{N}\left(\mathbf{p}_i^2 - \frac{\alpha Z}{r_i}\boldsymbol{\alpha}_i\cdot\mathbf{p}_i - \frac{\alpha Z}{r_i}\left(\boldsymbol{\alpha}_i\cdot\mathbf{C}_i^1\right)\mathbf{C}_i^1\cdot\mathbf{p}_i\right)$$

$$H_{\mathrm{SMS}} = \frac{1}{2M}\sum_{i\neq j}^{N}\left(\mathbf{p}_i\cdot\mathbf{p}_j - \frac{\alpha Z}{r_i}\boldsymbol{\alpha}_i\cdot\mathbf{p}_j - \frac{\alpha Z}{r_i}\left(\boldsymbol{\alpha}_i\cdot\mathbf{C}_i^1\right)\mathbf{C}_i^1\cdot\mathbf{p}_j\right)$$


F = -772 MHz/fm2, IS(65-63) = 576.1 MHz
M (GHz amu)
1500
1400
1300
1200
1100
1000
900
μ window
ES window
S. Fritzsche
relativistic operators
T + Hsms 1
29000
29500
30000
30500
ν̃exp
31000
E (cm-1)



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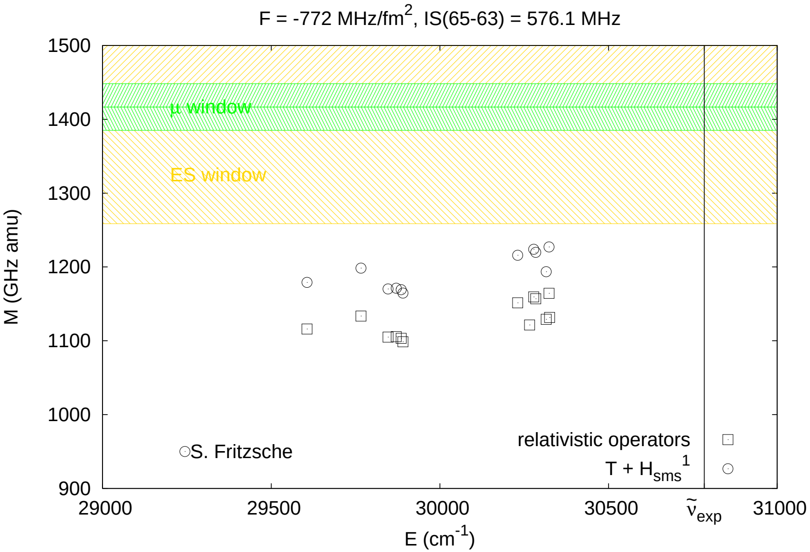
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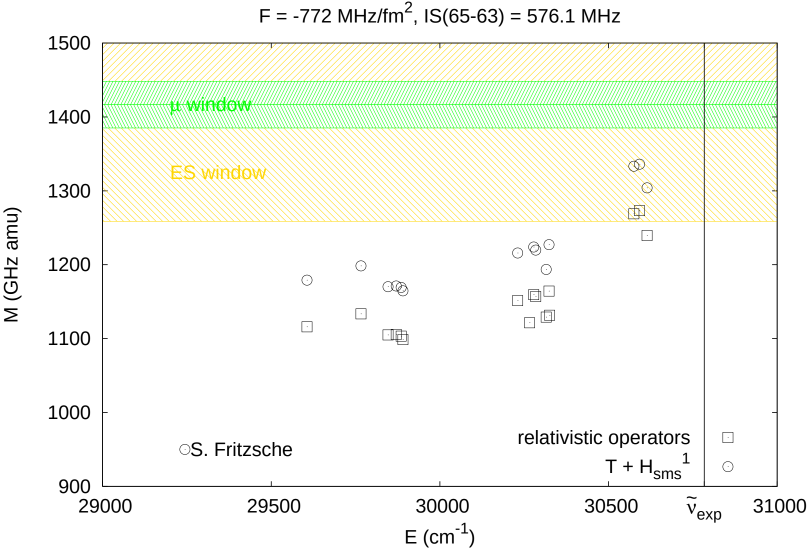
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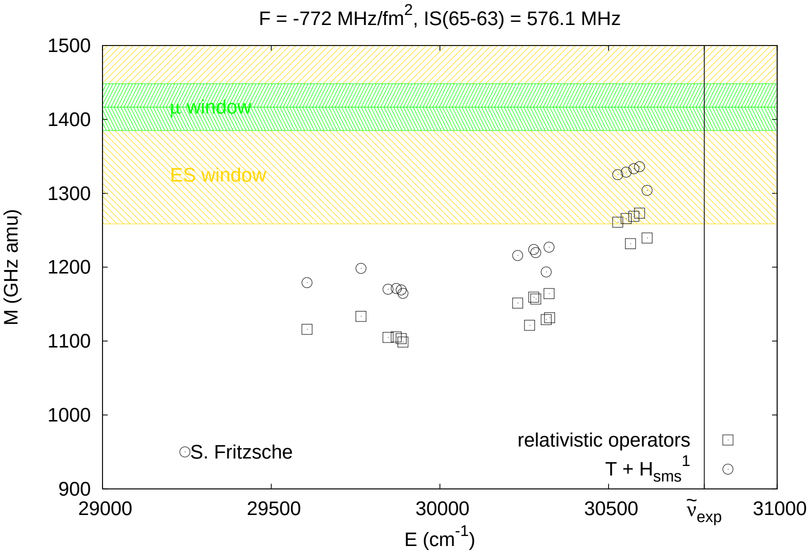
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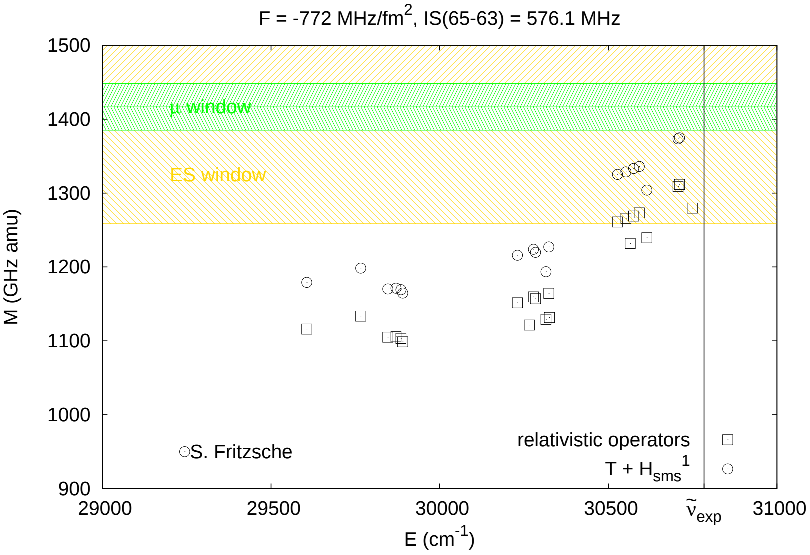
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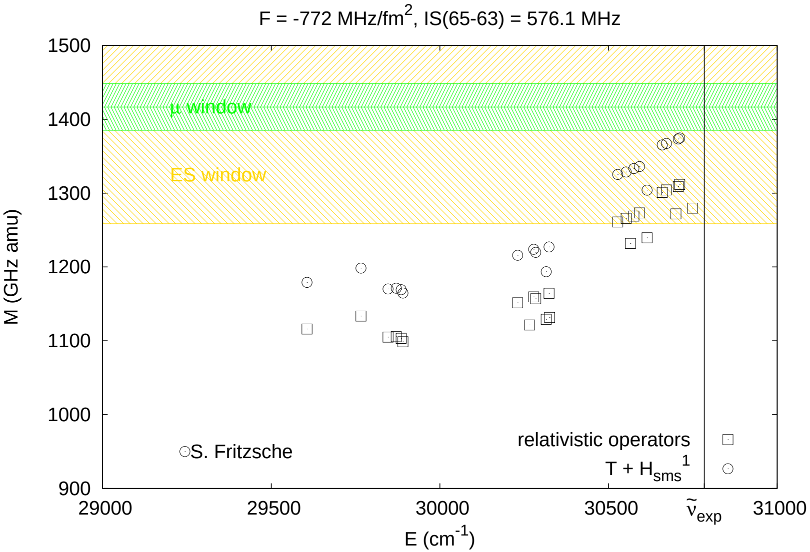
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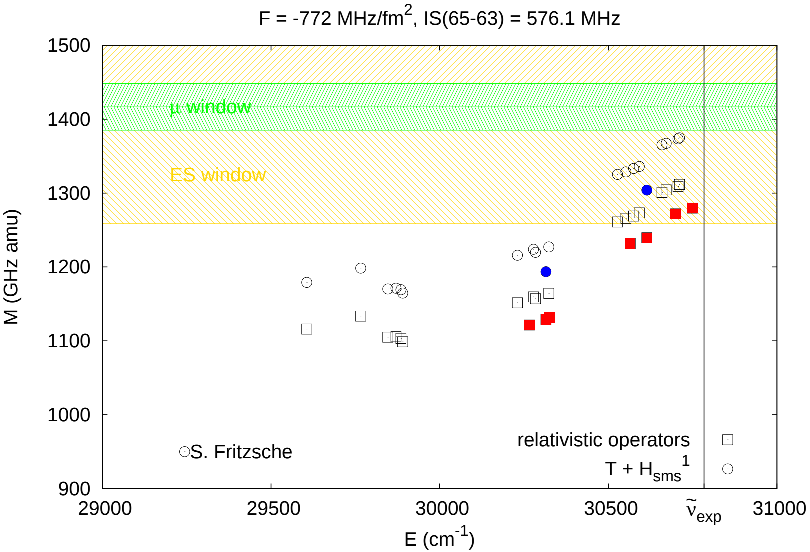
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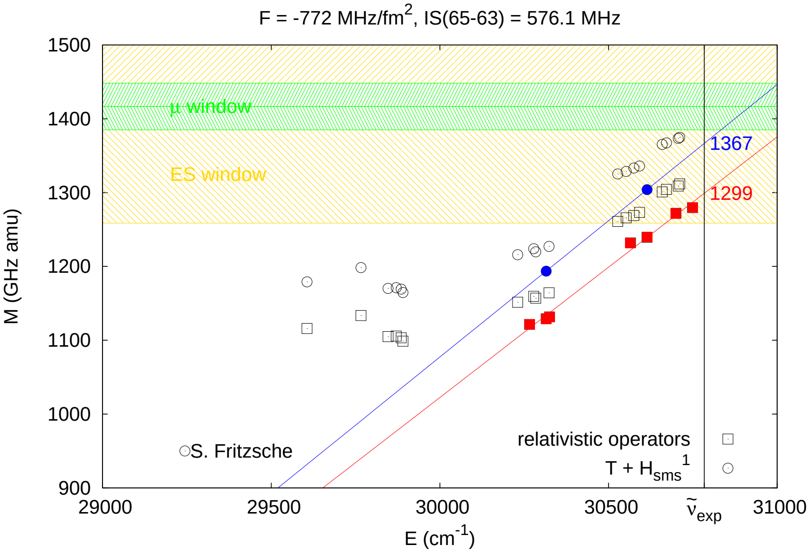
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900
M (GHz amu)
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1299
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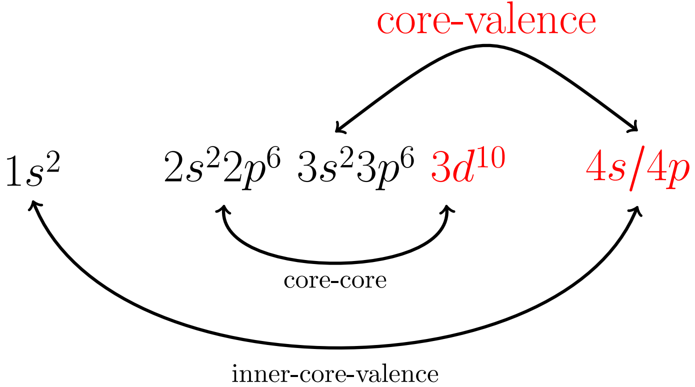
core-valence
1s2
2s22p6 3s23p6 3d10
4s/4p
core-core
inner-core-valence

Thanks